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Study Optical Properties Of Organic Thin Films And Its Application On Solar Cell

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Abstract

Several advantages are available with organic semiconductors, including easy synthesis, straightforward purification, high solubility, inexpensive manufacture, and significant industrial significance. Therefore, materials for large-scale electrical and optoelectronic devices made of organic semiconductors show promise. Therefore, studying the optical properties of these materials is very important not only for designing the devices, but also for knowing their absorption limits, determine the type of optical transition and the optical energy gap value to assess their viability for solar cell fabrication. For instance, we investigated the optical characteristics of thin films of 4-dimethylaminobenzylidenemalononitrile (DBM). Through the process of thermal evaporation, the (DBM) thin films were created. Deposition was carried out on clean optical flat fused quartz substrates for optical measurements at room temperature and at two different thermal annealing temperatures of 323 and 373 K. Using a double-beam

spectrophotometer, the transmittance T(λ) and reflectance R(λ) of DBM thin films with a thickness of 480 nm were measured in the 200–2500 nm spectral region. It is possible to determine the absorption index (k) and refractive index (n). Calculations were made for the optical energy gap and Urbach energy at ambient temperature as well as at various thermal annealing temperatures (323 and 373K). It was found that the indirect energy gap increases with increasing thermal annealing from 0.9325 eV for thin film as – deposited to 0.9575 eV at 373. The optical characteristics of DBM films can be changed by thermal annealing, which has numerous significant uses, including high-capacity communications networks.. This means that the material is suitable for use in manufacturing solar cells.

Key Words:Optical constants, Refractive index, Absorption index,Thermal annealing.

1. Introduction:

As a renewable and sustainable energy source, solar cells are crucial. Because it has many advantages, including the ability to use sunlight to generate electricity, lower greenhouse gas emissions, reduce the effects of climate change, promote energy independence, save costs in the long term, provide a clean environment, and reduce the need for fossil fuels. It also makes remote power generation possible and can be easily scaled up or down to accommodate varying power requirements [1,2] . Because of their adjustable optical, electrochemical, and electrical properties, organic semiconductor materials have seen a major increase in development for optoelectronic and photonic applications in recent years [3]. Numerous benefits come with this kind of organic semiconductor, including inexpensive manufacturing costs, good solubility, straightforward synthesis, straightforward purification, intriguing unique features, and significant industrial significance [4]. Literature has therefore sprung up around the theme. Promising materials for large-scale electrical and optoelectronic devices are organic semiconductors [4]. Researchers and engineers are making many new advances in device technology by studying the optoelectronic properties of organic semiconductors suitable for many applications [5]. There is currently a growing market for organic materials used in new applications for solar cell devices [6]. Thin-film organic semiconductors were employed by numerous researchers in a variety of applications to enhance film preparation techniques. thus, it is necessary to know the relationships between many of the controlling properties of the organic semiconductor films [7]. One of these organic compounds is 4-dimethylaminobenzylidenemalononitrile, abbreviated DBM.There are several techniques for growing DBM layers such as a pulsed laser deposition (PLD) method [8], the epitaxial layers were grown from solution [9], Molecular beam epitaxy (MBE) growth [10],and also by thermal evaporation technique[11]. The most significant aspect of organic materials is the facile production process utilizing low-cost technologies by thermal evaporation in comparison with inorganic materials [12]. DBM dye is a novel family of organic semiconducting materials that can be utilized for manufacturing D/A solar cells [13].

Optical properties of (DBM) thin films have been investigated to determine their suitability in manufacturing solar cells.

2. The Theoretical Framework

The following formulas was used to obtain the extinction coefficient (k), absorption coefficient (α), and refractive index (n) using the values of T (λ) and R (λ) at room temperature and different thermal annealing temperatures [14].

$$\alpha = \frac{1}{d} ln \left[\frac{(1-R)^2}{2T} + \frac{(1-R)^4}{4T^2} + R^2\right]^{1/2} \qquad (1)$$

The extinction index k can be obtained from the following expression [14]:

$$k = \alpha\lambda / 4\pi \qquad (2)$$

The refractive index can be extracted using the following Eq. [14-16]:

$$n = \left(\frac{1+R}{1-R}\right) + \sqrt{\frac{4R}{(1-R)^2} - k^2}, \qquad (3)$$

The width of the localized states influencing the optical band gap structure and optical transitions is known as the Urbach tail. Urbach's energy, Eu, values for DBM films can be determined by [17]:

$$ln(\alpha) = ln(\alpha_0) - (h\upsilon/E_u) \qquad (4)$$

Where α is the absorption coefficient, which may be found from k values, and E_u is the width of the tail of localized states in the forbidden band gap, $\alpha_0$is a constant [18]. The following formula uses the Tauc's relationship to find the optical band gap, E_g, values and the type of optical transition[19]:.

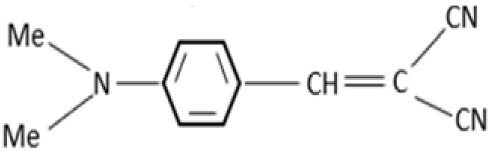
$$(\alpha h\upsilon)^m = A(h\upsilon - Eg), \qquad (5)$$

Where A is a constant and m is an index representing the type of transition, which can take values of 2, 1/2 in the case of direct and indirect allowed optical transitions, respectively.

3. Experimental process

3.1. Material under investigation

4-dimethylaminobenzylidenemalononitrile (DBM) used in this work was experimentally prepared by a chemical reaction between 4-dimethyl amino benzaldehyde and malononitrile in ethanol. The mixture was heated for 30 minutes, and then it was cooled to room temperature. Yellow crystals were formed which were then filtered from ethanol N. A. Elsayed et al [20]. The molecular structure diagram of. (DBM) is demonstrated in Scheme. 1.



Scheme 1.Molecular structure diagram of 4–dimethylaminobenzylidenemalononitrile

DBM has a molecular weight of 197.24 and the chemical formula $C_{12}H_{11}N_3$..DBM thin films have been prepared using a coating device (Edwards type E306A, England) and the thermal evaporation method under a vacuum of roughly 10^{-5} Pa.

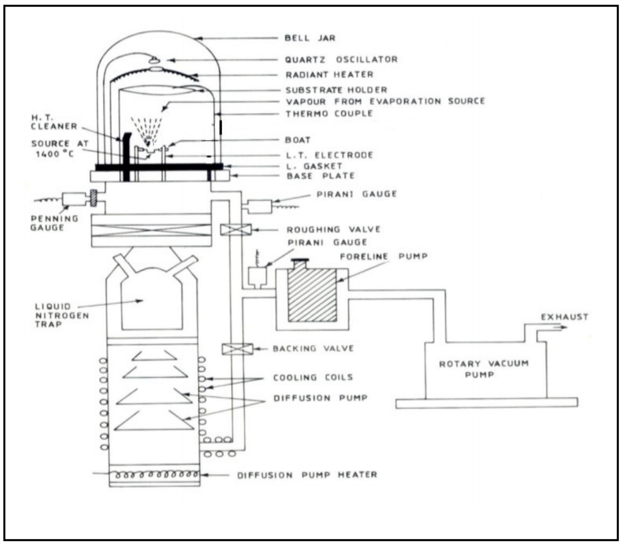


Figure 1: A schematic diagram of the vacuum and evaporation system

The thermal evaporation technique is one of the simple methods to use of controlling the parameters of the deposition, like the substrate temperature, the thickness of the film, evaporation rate. The deposition rate was controlled at 2.5 nm s $^{-1}$.The depositions were made at room temperature and different thermal annealing temperatures at 323 and 373 K for Two hours on to clean optical flat fused quartz substrates for optical measurements. A quartz crystal thickness monitor was used to calculate the film thickness (FTM4, Edwards),the thin–film thickness DBM is (480 nm).The transmittance T (λ) and reflectance R (λ) from 200 to 2500 nm at room temperature and various thermal annealing temperatures were measured using a spectrophotometer (JASCO V–570, UV–visible–NIR). The annealing was carried out for two hours at 323 and 373K.

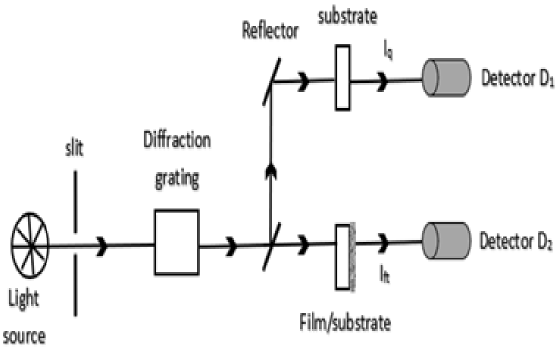


Figure 2: *Schematic diagram showing the spectrophotometer (T–mode)*

4. Results of Research

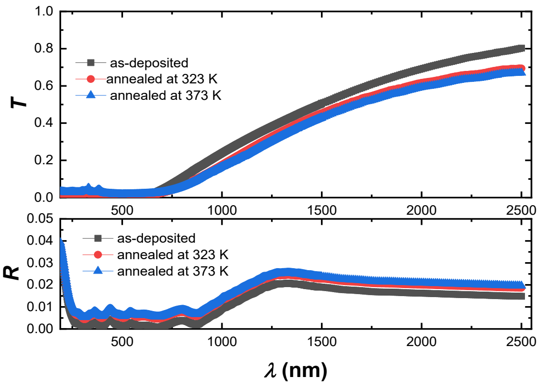


Figure (3): The transmittance T(λ) and reflectance R(λ) for DBM films that were as-deposited and annealed for two hours at 323 and 373 K with a thickness of 480 nm.

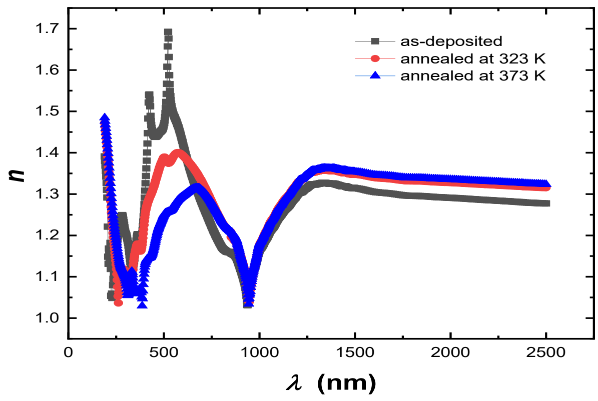


Figure (4): The refractive index (n) spectrum behavior of DBM films as- deposited and annealed at (323 and 373 K)..

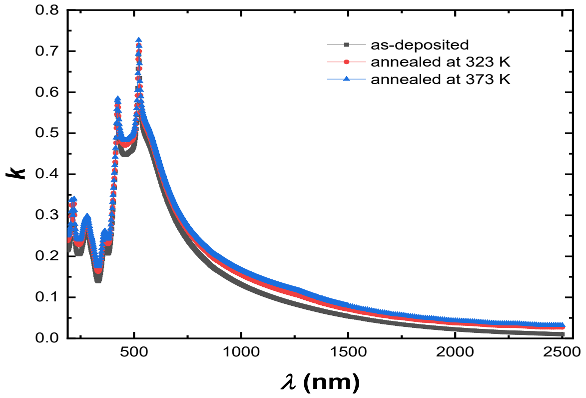


Figure (5): The spectral behavior of absorption index, k for DBM as- deposited and annealed films at (323 and 373 K).

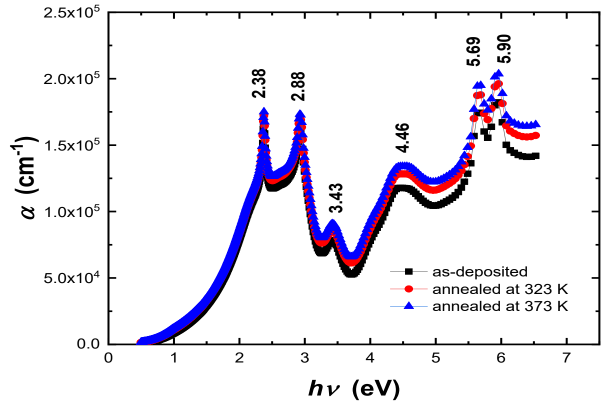


Figure (6): The absorption coefficient's spectrum behavior α for as- deposited and annealed films at (323 and 373 K).

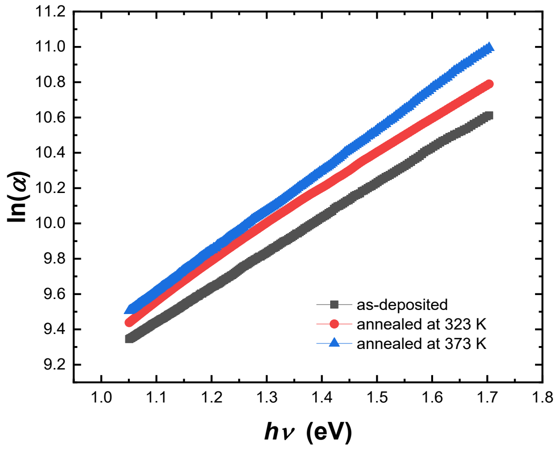


Figure (7): Plot of ln(α) against hυ for DBM as-deposited and annealed films at (323 and 373 K).

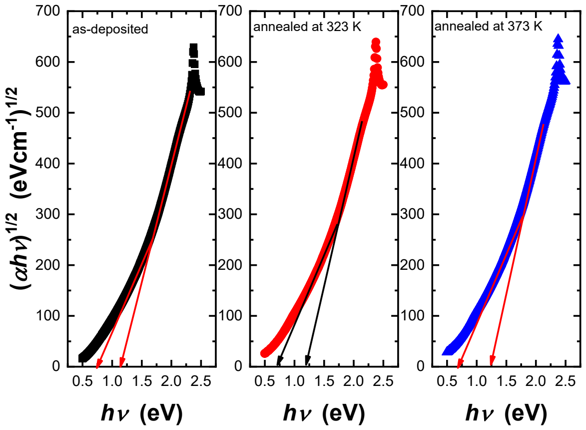


Figure (8): Plot of (αhυ) $^{1/2}$ against hυ for as-deposited and annealed films at (323 and 373 K).

Table (1): Values of E_u and E_g^{ind} for as–deposited and annealed films.

Sample	E_g^{ind} **(ev)**	E_{ph} **(mev)**	E_u **(ev)**
as–deposited	**0.9325**	**257.5**	**0.5**
annealed at 323 K	**0.9429**	**226.9**	**0.458**
annealed at 373 K	**0.9575**	**192.5**	**0.44**

5. Interpretation of Results

5.1 Optical characteristics of DBM films as-deposited and after annealing

T (λ) and R (λ) spectra of 480 nm thick DBM thin films as-deposited and annealed films at various temperatures (323 and 373K) for 2 hours were obtained in the 200–2500 nm range, as shown in Fig. 3. It is observed that there is a transmittance edge separating between two regions. The first region at wavelengths (< 700 nm) is called the absorbing region, at which (i.e. $R + T + S \neq 1$). The second region at wavelengths (>700 nm) is known as the non-absorbing region, at which light is scattered or transmitted ($R + S + T \approx 1$). The presence of such an edge in the spectra indicates that this material is used as a good optical filter material. The absence of ripples in the spectral behavior suggests that the films are uniformly thick and homogenous. The annealed film's optical transmittance edge is observed to gradually move towards lower wavelengths, indicating that the annealing impact will increase the optical energy band gap.

The DBM thin-film spectral behaviors of n and k as deposited and annealed films at various temperatures (323 and 373K) for two hours, of thickness 480 nm measured from equations (2 and 3) are shown in Figures 4 and 5, respectively. It is observed that the dispersion curve contains two regions (anomalous and normal) [21].

The results of calculations showed that the optical constants are independent of film thickness where the variation was found to be within the experimental errors.

5.2. Urbach energy and optical energy gap

As we have previously stated, the Urbach tail represents the width of local states influencing optical transitions and the optical band gap. For DBM films, the values of E_u, Urbach's energy, are calculated using equation (4). Figure 6 shows the values of α for a 480 nm thick DBM thin film that has been deposited and annealed, as a function of photon energy, $h\upsilon$. It is evident that the absorption coefficient ranges from 10^5 cm^{-1}. It is also evident that after annealing, the absorption coefficient increases slightly. [22]. Figure 7 shows a linear relationship for both as-deposited and annealed DBM films between the photon energy, $h\upsilon$, and the natural logarithm of the absorption coefficient, $\ln(\alpha)$. The reciprocal of each line's slope yields the magnitude of E_u,and its values are listed in Table 1. We can show that the annealing process decreases the Urbach energy of DBM film.

To know the type of optical transition and calculate the optical band gap, we use the Tauc's relationship equation (5).The experimental data have been fitted with the theoretical equation (5) for different values of m. The best fit was obtained for m = 1/2 indirect allowed transitions, which are presented by the next modified equation [23, 24].

$$(\alpha h\upsilon)^m = A(h\upsilon - E_g \pm E_{ph}) \qquad (6)$$

Where E_{ph} is the energy of phonons-assisted indirect allowed transition

Fig.8 illustrates the functional dependence of $(\alpha h\upsilon)^{1/2}$ on $h\upsilon$ for as-deposited and annealed film of thickness 480 nm.

The obtained values of indirect band gap (E_g^{ind}) and energy of phonons (E_{ph}) from these curves are listed in Table 1. It is demonstrated that as the thermal annealing temperature rises, the optical energy gap grows. The optical band gap represents a significant application in ascertaining the energy gap between the top valance band and the bottom conduction band of the materials under investigation [25, 26].

A DBM/n-Si hybrid organic-inorganic solar cell was fabricated. The rectification ratio (RR) value at +1 V was calculated and equals 4043.5. It is clear that the measured cell showed strong corrective behaviour. The DBM/n-Si cell has an efficiency of 1.48% and a fill factor (FF) of 0.361 under illumination. [20].

6. Conclusion

The optical properties of thin films (DBM) fabricated by thermal evaporation process on a quartz substrate were studied at room temperature and at different thermal annealing temperatures of 323 and 373 K. The optical study showed that the annealing process increases the indirect energy gap, decreases the energy of phonons and the Urbach energy with annealing temperatures. These findings suggest that thermal annealing has an impact on paramaters. that may be reflected in the thermodynamic stability of the tested materials. Thus, the suitability of annealed films (DBM) for optoelectronic device applications such as hybrid organic-inorganic solar cells has been confirmed.

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